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Stereochemistry of seven-membered heterocycles Communication 16. Dipole moments, IR,1H, and13C NMR spectra, and conformations of 4-methyl-, 4-phenyl-, and isomeric 4,7-dimethyl-2,2-pentamethylene-1,3-di0-a-5,6-benzocycloheptenes

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Abstract

1. 1H NMR,13C NMR, and IR spectroscopy and dipole moment measurements showed that the conformational mobility of 4-methyl-, 4-phenyl-, and trans-4,7-dimethyl-2,2-pentamethylene-1,3-dioxa-5,6-benzocycloheptenes is a consequence of the cyclohexane ring with rigid twist conformation of the heterocycle. The NMR signals of the benzyl protons of the heterocycle were assigned. 2. The corresponding cis isomer exists as a conformational mixture of chair and twist forms. © 1985 Plenum Publishing Corporation.

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